Numerical homogenization of geometric network models

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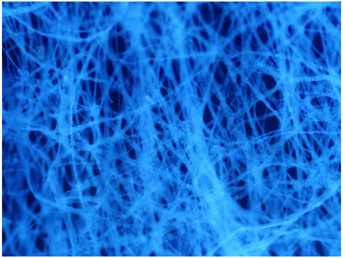
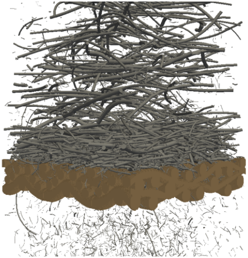
Motivation: Numerical simulation of paper



- Fraunhofer Chalmers Centre (paper making, properties)
- Stora Enso and Albany International
- Gustav Kettil, PhD 2014-2019, (Chalmers/FCC)
- Scientific advisor at FCC 2018-ongoing
- Morgan Görtz, PhD 2019- (Chalmers/FCC, SSF)

Motivation: Numerical simulation of paper



▷ fluid-structure interaction

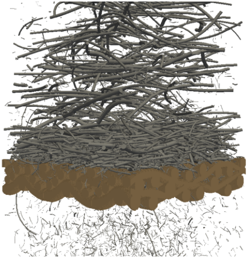
▷ elastic network model

ISOP project:

- Simulate the paper making process
- Simulate the finished product (tensile, bending, defects)
- Optimize (fiber dimensions, distribution, fabric)

Numerical simulation is not used extensively

Motivation: Numerical simulation of paper



▷ fluid-structure interaction

▷ elastic network model

Morgan's project:

- Large (A4) scale simulation (periodically expand 9mm $\times$ 9mm)
- Tensile and bending strength, crack propagation
- Offline-online setting (numerical homogenization)

From mathematical analysis to software used by companies.

Outline

Homogenization in 1D

Consider

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left(A_\epsilon(x)\frac{\mathrm{d}}{\mathrm{d}x}u_\epsilon(x)\right) = f(x), \quad \text{in } \Omega = [0,1]$$

where $A_\epsilon = A(x/\epsilon)$ periodic with period ϵ.

Then $u_\epsilon \to u_0$ in $L^2([0,1])$ where

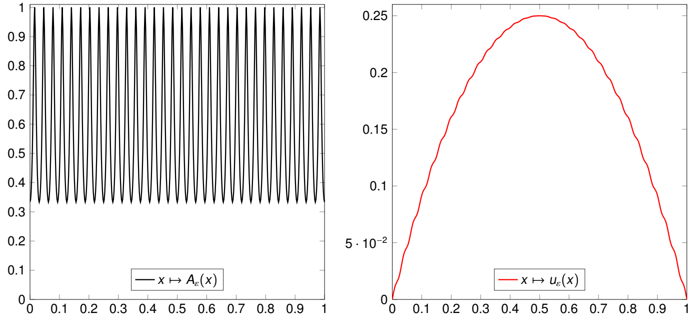
$$-\frac{\mathrm{d}}{\mathrm{d}x}\left(A^*\frac{\mathrm{d}}{\mathrm{d}x}u_0(x)\right) = f(x), \quad \text{in } [0,1]$$

where the effective diffusion A^* is the harmonic mean

$$A^* = \left(\frac{1}{\epsilon}\int_{I_\epsilon} A(x/\epsilon)^{-1}\,\mathrm{d}x\right)^{-1}$$

FEM for periodic problem

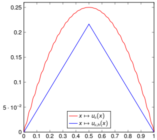
Let $A_\epsilon = (2 + \cos(2\pi x/\epsilon))^{-1}$ with harmonic mean $\frac{1}{2}$ if $\epsilon^{-1} \in \mathbb{N}$.



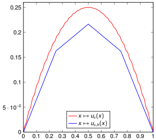
FEM: Find $u_{\epsilon,h} \in V_h \subset V = H_0^1(\Omega)$ such that

$$\int_\Omega A_\epsilon u_{\epsilon,h}' v' \,\mathrm{d}x = \int_\Omega f\, v \,\mathrm{d}x, \qquad \forall v \in V_h.$$

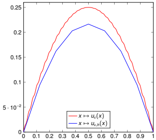
FEM for periodic problem $\epsilon = 2^{-5}$



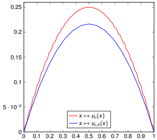
(a) $h = 2^{-1}$.



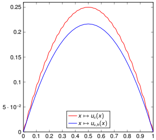
(b) $h = 2^{-2}$.



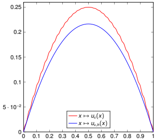
(c) $h = 2^{-3}$.



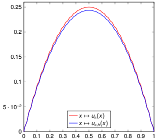
(d) $h = 2^{-4}$.



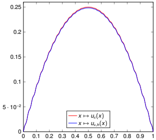
(e) $h = 2^{-5}$.



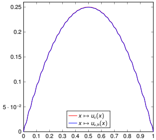
(f) $h = 2^{-6}$.



(g) $h = 2^{-7}$.



(h) $h = 2^{-8}$.



(i) $h = 2^{-9}$.

FEM for periodic problem

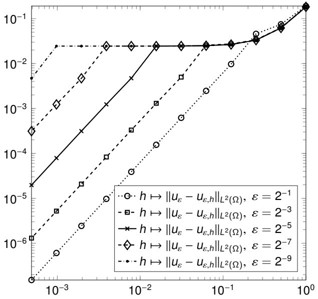


Figure: $\|u_{\epsilon,h} - u_\epsilon\|_{L^2(\Omega)}$ vs. h for several values of ϵ.

FEM sees the average coefficient $\bar{A}_\epsilon = \frac{1}{\sqrt{3}} \neq \frac{1}{2}$ when $h > \epsilon$

$$\int_\Omega A_\epsilon u'_{\epsilon,h} v' \, \mathrm{d}x = \sum_{T \in \mathcal{T}_h} u'_{\epsilon,h} v' \int_T A_\epsilon \, \mathrm{d}x = \int_\Omega \bar{A}_\epsilon u'_{\epsilon,h} v' \, \mathrm{d}x$$

Numerical homogenization in 1D

Assume non-periodic diffusion:

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left(A(x)\frac{\mathrm{d}}{\mathrm{d}x}u(x)\right) = f(x), \quad \text{in } \Omega = (0,1)$$

- There is no constant A^*.
- Can we find V_H^{ms} with $\dim(V_H^{\mathrm{ms}}) = \dim(V_H)$ and achieve

$$\|u - u_H^{\mathrm{ms}}\|_{L^2(\Omega)} \leq CH^2\|f\|_{L^2(\Omega)}$$
$$\|u - u_H^{\mathrm{ms}}\|_{H^1(\Omega)} \leq CH\|f\|_{L^2(\Omega)}$$

  for all $H > 0$?
- Can we find a local basis of V_H^{ms}?

Numerical homogenization in 1D

Let $V_H = P1(\mathcal{T}_H) \subset V$ continuous piecewise affine and $V = H_0^1(\Omega)$.
Let $I_H : V \to V_H$ be the nodal interpolant and define

$$W = \{v \in V : I_H v = 0\} = \ker(I_H)$$

We note that

$$\int_\Omega v_H' w' \,\mathrm{d}x = \sum_{T \in \mathcal{T}_H} (v_H'|_T) \int_T w' \,\mathrm{d}x = 0$$

V_H and W are orthogonal wrt $(v', w') = \int_\Omega v' w' \,\mathrm{d}x$ and
$V = V_H \oplus W$.

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V_H and W are orthogonal wrt $(v', w') = \int_\Omega v' w' \,\mathrm{d}x$ and $V = V_H \oplus W$.
We instead use the bilinear form to construct $V = V_H^{\mathrm{ms}} \oplus W$ with

$$V_H^{\mathrm{ms}} = \{v \in V : \int_\Omega A v' w' \,\mathrm{d}x = 0, \quad \forall w \in W\}$$

Numerical homogenization in 1D

We have that $u \in V$ and $u_H^{\mathrm{ms}} \in V_H^{\mathrm{ms}}$ solves

$$\int_\Omega A u' v' \,\mathrm{d}x = \int_\Omega f v \,\mathrm{d}x, \qquad \forall v \in V$$
$$\int_\Omega A (u_H^{\mathrm{ms}})' v' \,\mathrm{d}x = \int_\Omega f v \,\mathrm{d}x, \qquad \forall v \in V_H^{\mathrm{ms}}.$$

Furthermore $u = u_H^{\mathrm{ms}} + u_w$ with $u_w \in W$. Coercivity, interp., C-S

$$\alpha \|u_w'\|^2_{L^2(\Omega)} \leq \|A^{1/2} u_w'\|^2_{L^2(\Omega)} = \int_\Omega A u_w' u_w' \,\mathrm{d}x = \int_\Omega A u' u_w' \,\mathrm{d}x$$
$$= \int_\Omega f\, u_w \,\mathrm{d}x \leq \|f\|_{L^2(\Omega)} \|u_w - I_H u_w\|_{L^2(\Omega)} \leq CH \|f\|_{L^2(\Omega)} \|u_w'\|_{L^2(\Omega)}$$

and therefore $\|u - u_H^{\mathrm{ms}}\|_{H^1(\Omega)} \leq CH \|f\|_{L^2(\Omega)}$.

Numerical homogenization in 1D

We let $V_H = \text{span}(\{\Lambda_j\}_{j=1}^n)$ and define

$$V_H^{\text{ms}} = \text{span}(\{\Lambda_j^{\text{ms}} := \Lambda_j - Q\Lambda_j\})$$

where $Q\Lambda_j \in W$ solves

$$\int_\Omega A(Q\Lambda_j)' w' \mathrm{d}x = \int_\Omega A\Lambda_j' w' \mathrm{d}x, \quad \forall w \in W$$

i.e. $\int_\Omega A(\Lambda_j - Q\Lambda_j)' w' \mathrm{d}x = 0$ for all $w \in W$.

Numerical homogenization in 1D

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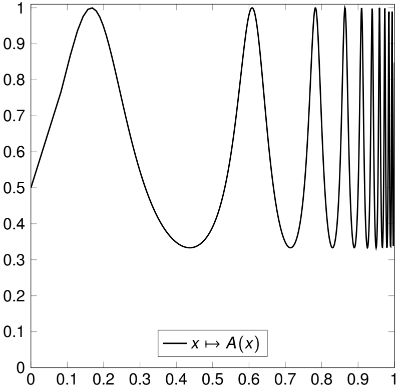
i.e. $\int_\Omega A(\Lambda_j - Q\Lambda_j)'w'\mathrm{d}x = 0$ for all $w \in W$.

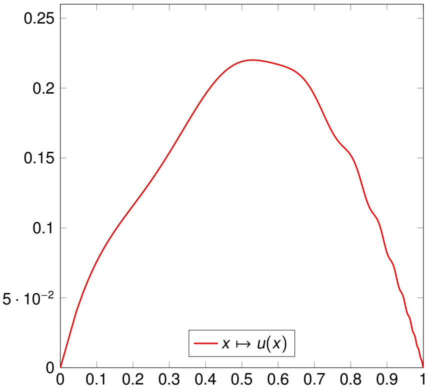
$$\Lambda_j^{\text{ms}}(x) := \begin{cases} \dfrac{\int_{x_{j-1}}^{x} A^{-1}(s)}{\int_{x_{j-1}}^{x_j} A^{-1}(s)}, & \text{if } x \in [x_{j-1}, x_j], \\ 1 - \dfrac{\int_{x_j}^{x} A^{-1}(s)}{\int_{x_j}^{x_{j+1}} A^{-1}(s)}, & \text{if } x \in [x_j, x_{j+1}], \\ 0, & \text{else.} \end{cases}$$

Numerical homogenization in 1D

Let $A = (2 - \sin(2\pi \tan(15\pi x/32)))^{-1}$ and $f = 1$.



(a)



(b)

Numerical homogenization in 1D

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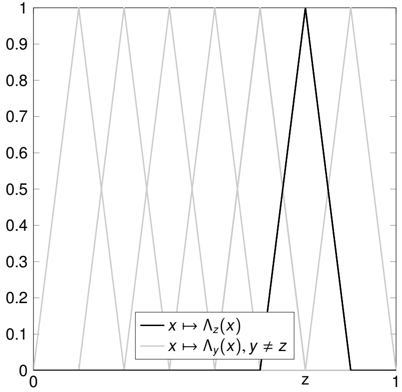
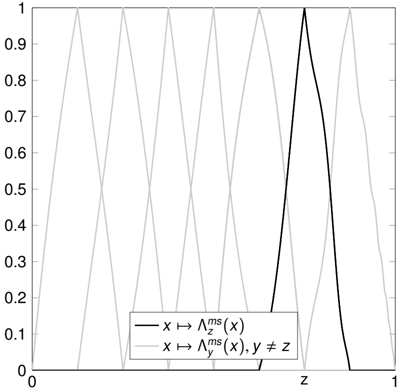


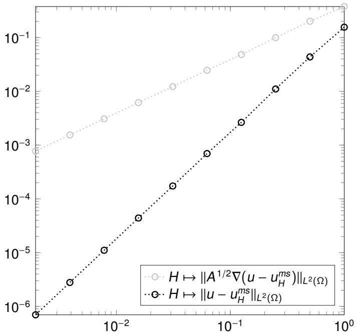
(c) Classical nodal basis Λ_j.



(d) Corrected nodal basis Λ_j^{ms}.

Numerical homogenization in 1D

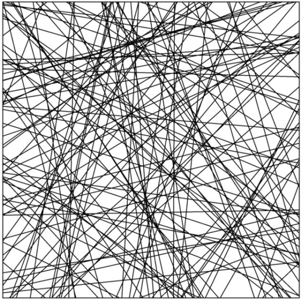
Let $A = (2 - \sin(2\pi \tan(15\pi x/32)))^{-1}$ and $f = 1$.



- Many approaches leads to this LOD, VMS, MsFEM,...
- LOD works in 2D, 3D. Non-local basis, no explicit formula!

M. & Peterseim, *Numerical homogenization by LOD*, SIAM Spotlights 2020

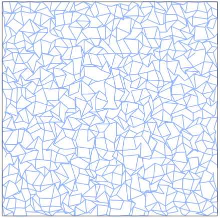
Numerical homogenization of a network?



- Example: Weighted graph Laplacian:
  $$L([i,j],[i,j]) := L([i,j],[i,j]) + a_{ij}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$
- Coarse scale (H) representation using LOD.
- Challenges: non-conforming, no Poincaré, interpolation, ...

Outline

A geometric network model



- Nodes $\{x_i\}_{i=1}^n \in \bar{\Omega}$ and edges $\{e_{ij}\}$.
- $V = \{v \in \mathbb{R}^n : v(x_i) = 0 \text{ for all } x_i \in \partial\Omega\}$
- $F \in V$
- $K : \mathbb{R}^n \to \mathbb{R}^n, \quad K = \sum_{i=1}^n K_i, \quad K_i$ SP(semi-)D

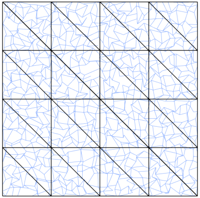
Find $u \in V$ such that

$$(v, Ku) = (v, F), \quad \forall v \in V$$

where $(v, w) = v^\top w$.

- We assume (v, Kv) to be coercive on V, i.e. we have a unique solution $u \in V$.
- For inhomogeneous bc let $u = u_0 + g$, $u_0 \in V$.

FE discretization



- $\mathcal{T}_H = \{T\}$, $H = \max \operatorname{diam}(T)$, quasi-uniform, shape regular $\frac{\operatorname{diam} B_T}{\operatorname{diam}(T)} \geq \rho$
- FEM space $S_H = \operatorname{span}(\{\Lambda_j\}_{j=1}^m)$, $\Lambda_j(y_i) = \delta_{ij}$
- $S_{H,0} = \{v \in S_H : v|_{\partial\Omega} = 0\} = \operatorname{span}(\{\Lambda_j\}_{j=1}^{m_0})$

We interpolate Λ_j onto the network to construct

$$\phi_j(x_i) = \Lambda_j(x_i), \quad 1 \leq j \leq m,\ 1 \leq i \leq n$$

and let $V_H = \operatorname{span}(\{\phi_j\}_{j=1}^{m_0}) \subset V$.

To each network node x_i we associate one element T, $x_i \in T$, and define

$$(v, w)_T = \sum_{x_i \in T} v(x_i) w(x_i).$$

Interpolation and decomposition

Scott-Zhang type interpolation operator $\mathcal{I}_H : V \to V_H$

$$\mathcal{I}_H v = \sum_{j=1}^{m_0} (\psi_j, v)_{T_j} \phi_j.$$

with $(\psi_j, \phi_i)_{T_j} = \delta_{ij}$ being the dual basis defined on an element T_j adjacent to j.

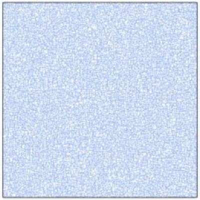
$$W = \ker(\mathcal{I}_H) \qquad V_H^{\text{ms}} = \{v \in V : (w, Kv) = 0 \ \forall w \in W\}.$$

By defining $Q : V \to W$ fulfilling

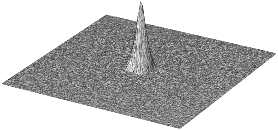
$$(w, KQv) = (w, Kv), \quad \forall w \in W$$

we can write $V_H^{\text{ms}} = (1 - Q)V_H$ and $V = V_H^{\text{ms}} \oplus W$.

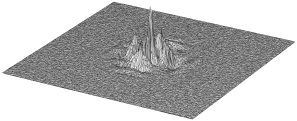
Example: A weighted graph Laplacian



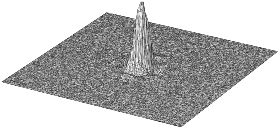
- Material parameter $\gamma_e > 0$, $K = \sum_e K_e$
- $K_{e_{ij}}([i,j],[i,j]) = K_{e_{ij}}([i,j],[i,j]) + \frac{\gamma_{e_{ij}}}{|e_{ij}|}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$
- $K = \sum_{i=1}^{n} K_i, \quad K_i = \frac{1}{2}\sum_{j:e_{ij}\neq\emptyset} K_{e_{ij}}$



ϕ_j

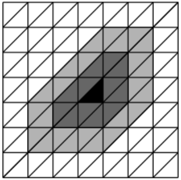


$Q\phi_j$



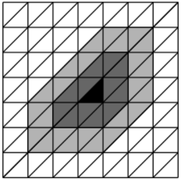
$\phi_j - Q\phi_j$

Localization



- $U^k(T) = U(U^{k-1}(T))$ with $U^0(T) = T$
- $W(U^k(T)) = \{w \in W : w(x_i) = 0 \; x_i \notin U^k(T)\}$
- $K_T = \sum_{x_i \in T} K_i$

Localization



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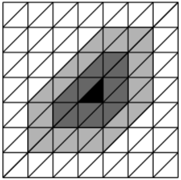
Find $Q_T^k v \in W(U^k(T))$ such that

$$(w, KQ_T^k v) = (w, K_T v), \quad \forall w \in W(U^k(T))$$

We let $Q^k = \sum_{T \in \mathcal{T}_H} Q_T^k$ and define $V_{H,k}^{\text{ms}} := (1 - Q^k) V_H$.

Localization



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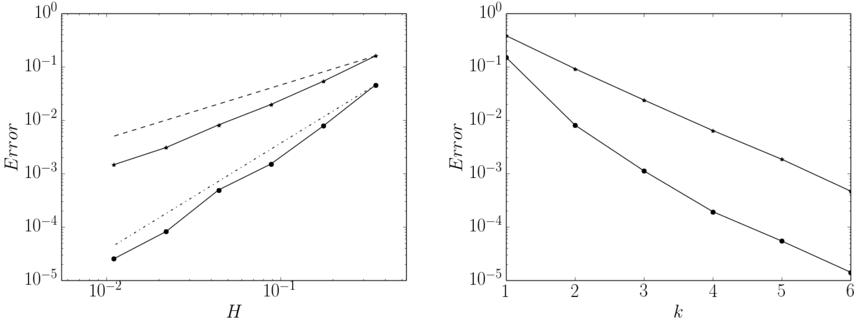
We let $Q^k = \sum_{T \in \mathcal{T}_H} Q_T^k$ and define $V_{H,k}^{\text{ms}} := (1 - Q^k) V_H$.

The LOD formulation reads: find $u_{H,k}^{\text{ms}} \in V_{H,k}^{\text{ms}}$ such that

$$(v, K u_{H,k}^{\text{ms}}) = (v, F), \quad \forall v \in V_{H,k}^{\text{ms}}$$

Example: A weighted graph Laplacian

We let F const, $\gamma_e \in [0.1, 1]$, and Dirichlet bc., quads $\mathcal{T}_H$.



Left: $k = \lceil \log(H^{-1}) \rceil$ Right: $H = 2^{-5}$

Relative errors in $\|\cdot\| = (\cdot,\cdot)^{1/2}$ and $|||\cdot||| = (\cdot, K\cdot)^{1/2}$.

Error analysis (weighted graph Laplacian)

- Poincaré inequality and interpolation bound:

$$\|v - \bar{v}\|_{L^2(\omega)} \leq C\mathrm{diam}(\omega)\|\nabla v\|_{L^2(\Omega)} \quad \forall v \in V$$

$$\lambda_2 := \inf_{w \in H_0^1(\Omega)\setminus\mathbb{R}} \frac{(\nabla w, \nabla w)_{L^2(\Omega)}}{(w, w)_{L^2(\Omega)}} \quad \rightarrow \quad \|v - \bar{v}\|_{L^2(\Omega)} \leq \lambda_2^{-1/2}\|\nabla v\|_{L^2(\Omega)}$$

If $\omega = [0, L]^2$ then $\lambda_2 = \frac{\pi^2}{L^2}$ i.e. $\lambda_2^{-1/2} \approx \mathrm{diam}(\omega)$

Error analysis (weighted graph Laplacian)

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$$\|v-\bar{v}\|_{L^2(\omega)} \leq C\mathrm{diam}(\omega)\|\nabla v\|_{L^2(\Omega)} \quad \forall v \in V$$

$$\lambda_2 := \inf_{w\in H^1_0(\Omega)\setminus\mathbb{R}} \frac{(\nabla w, \nabla w)_{L^2(\Omega)}}{(w,w)_{L^2(\Omega)}} \quad \rightarrow \quad \|v-\bar{v}\|_{L^2(\Omega)} \leq \lambda_2^{-1/2}\|\nabla v\|_{L^2(\Omega)}$$

  If $\omega = [0,L]^2$ then $\lambda_2 = \frac{\pi^2}{L^2}$ i.e. $\lambda_2^{-1/2} \approx \mathrm{diam}(\omega)$

- Fielder number: $\lambda_2 = \inf_{w\in V\setminus\mathbb{R}} \frac{w^TKw}{w^Tw}$ (algebraic connectivity).

Error analysis (weighted graph Laplacian)

- Poincaré inequality and interpolation bound:

$$\|v - \bar{v}\|_{L^2(\omega)} \leq C\mathrm{diam}(\omega)\|\nabla v\|_{L^2(\Omega)} \quad \forall v \in V$$

$$\lambda_2 := \inf_{w \in H^1_0(\Omega)\setminus\mathbb{R}} \frac{(\nabla w, \nabla w)_{L^2(\Omega)}}{(w, w)_{L^2(\Omega)}} \quad \rightarrow \quad \|v - \bar{v}\|_{L^2(\Omega)} \leq \lambda_2^{-1/2}\|\nabla v\|_{L^2(\Omega)}$$

  If $\omega = [0, L]^2$ then $\lambda_2 = \frac{\pi^2}{L^2}$ i.e. $\lambda_2^{-1/2} \approx \mathrm{diam}(\omega)$

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[3]Kornhuber et. al., *Numerical homogenization of elliptic multiscale problems by subspace decomposition*, SIAM MMS 2016

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Theorem

$$|||u - u_{H,k}^{ms}||| \leq C_1(H + exp(-C_2 k))||F||$$

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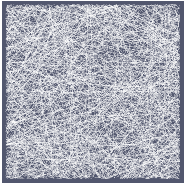
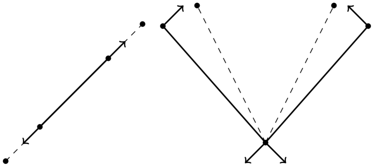
Outline

A fibre network model[4]



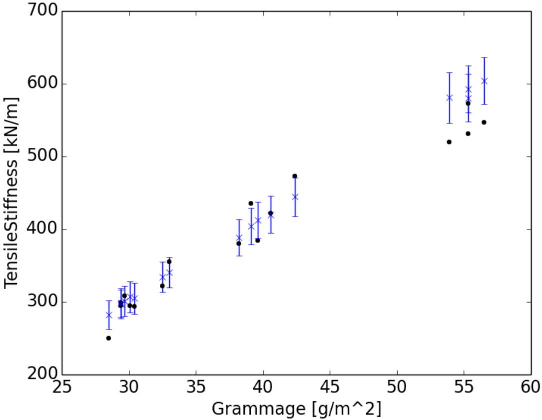


- Fibers are made of line segments in 3D, close lines are connected with bonds, the solution is the displacement
- Length 0.5 – 4mm, width 0.021 – 0.03mm, cross section $200(\mu\text{m})^2$
- Young's module of elasticity $E = 25$GPa.
- Two forces in the model: edge extension and angular deviation
- Edge pairs still allow $K = \sum_{i=1}^{n} K^i$, translations is in $\ker(K)$

[4]Kettil et. al. *Numerical upscaling of discrete network models*, BIT 2020

Validation with experiments

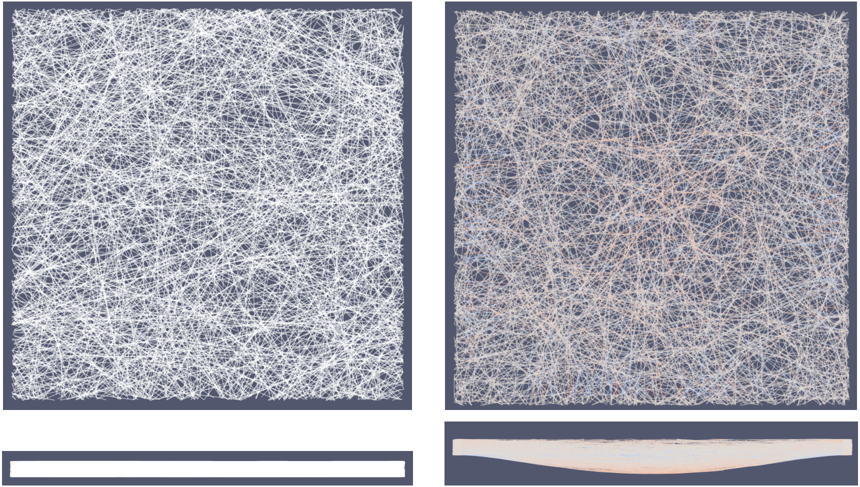
Clamped and pulled, randomly generated fibre configurations, mean and standard deviation.



Stiffness vs area density.

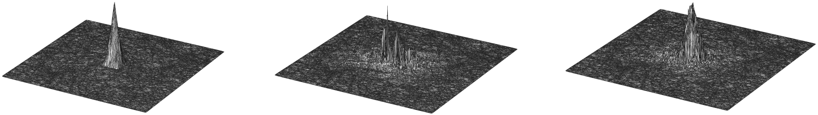
Example: LOD for fibre network model

Fixed boundary, constant force applied in all nodes.



Example: LOD for fibre network model

Similar localization as in LOD for linear elasticity[5].



[5] Henning et. al. CMAME 2016

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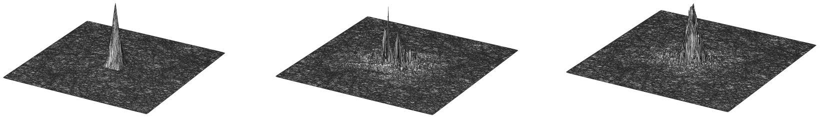
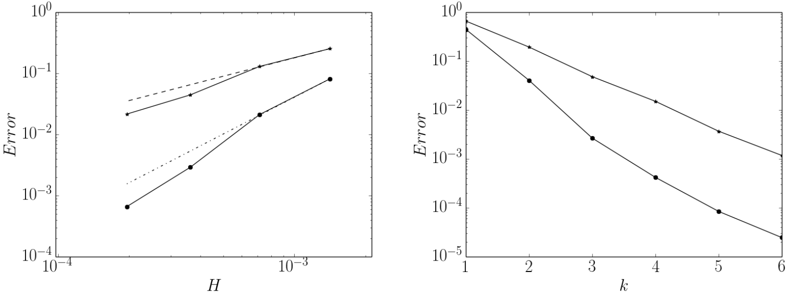


Relative errors ($\|\cdot\|$, $|||\cdot|||$). Left: $k = \lceil 1.5\log(H^{-1})\rceil$. Right: $H = 2^{-5}$.



[5]Henning et. al. CMAME 2016

Outline

1. Review of elliptic homogenization in 1D
2. Numerical homogenization of a network model
3. Fiber network model of paper
4. **Future work**

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Ongoing:

- Complete error analysis (Hellman)
- Scale up siumulation using periodicity (Görtz, Kettil)

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- Complete error analysis (Hellman)
- Scale up siumulation using periodicity (Görtz, Kettil)

Early stages:

- Defects and cracks, reuse of basis locally (Görtz, Kettil)
- Elastic wave propagation (Persson)
- Algebraic LOD (Hellman, Maier)

Thank you!